Work fluctuations for a Brownian particle between two thermostats

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Abstract. We explicitly determine the large deviation function of the energy flow of a Brownian particle coupled to two heat baths at different temperatures. This toy model, initially introduced by Derrida and Brunet [1], allows not only to sort out the influence of initial conditions on large deviation functions but also to pinpoint various restrictions bearing upon the range of validity of the Fluctuation Relation.

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The recent upsurge of interest in nonequilibrium statistical mechanics lies in the discovery of simple yet generic results, embodied by the Fluctuation Relation initially brought forth by Evans, Cohen and Morriss [2], and later formalized into a theorem by Gallavotti and Cohen [3]. This Fluctuation Relation states that in the nonequilibrium steady-state of a (chaotic, Anosov) dynamical system, the temporal large deviation function of an appropriately defined entropy current verifies a particular symmetry property under time reversal. In practice the latter entropy current consists of a heat or particle flux and could be accessed experimentally in some situations [4]. Before going into the specifics of that relation, we mention that a Markov dynamics analog of the Gallavotti-Cohen theorem was then found by Kurchan [5] and Lebowitz and Spohn [6]. More recently, other contributions on the subject have been put forward by Van Zon and Cohen [7], and by Bonetto *et al.* [8], where an extension of the Fluctuation Relation to quantities other than the entropy flux is proposed.

The purpose of the present report is to present a simple model for which nonequilibrium fluctuations can be investigated precisely at finite times. We will show that a seemingly innocuous initial condition dependence restricts the domain of validity of the Fluctuation Relation, even though the latter applies to asymptotic times.

In order to illustrate our point, we exploit a toy model introduced by Derrida and Brunet in a recent pedagogical account [1]. After having described this model, we will recall the standard statement of the Fluctuation Relation, and then we shall show that some initial condition effects, that intuition suggests to discard, can lead to an actual failure of the Fluctuation Relation.

We take a particle in contact with two heat baths imposing distinct temperatures T_1 and T_2, whose velocity $v(t)$ evolves according to the Langevin equation

$$m\dot{v} = -(\gamma_1 + \gamma_2)v + \xi_1(t) + \xi_2(t) \ , \tag{1}$$

with $\langle \xi_i \rangle = 0$ and

$$\langle \xi_i(t)\xi_j(t') \rangle = 2\gamma_i T_i \delta_{ij}\delta(t-t') = 2D_i\delta_{ij}\delta(t-t') \ , \tag{2}$$

where the Boltzmann's constant has been taken equal to one. Such an equation can also describe the dynamics of apparently different models, for example, the dynamics of a hard rod connected at both ends to two heat baths (as a slight variation of the model introduced in [9], and is sketched in Fig 1). We also note that another model, consisting of two overdamped brownian particles interacting with a harmonic potential [10, 11], can be exactly mapped on Eq. (1). Finally, we quote that other analogies in term of electric circuits, in the spirit of [12] can also be described by a Stochastic differential equation of the same type. Strictly speaking, the dynamics of the particle is an equilibrium one, since in Eq. (1) the sum of the Gaussian noises is another Gaussian noise with viscosity $\gamma = \gamma_1 + \gamma_2$ and noise strength $D = D_1 + D_2$. The velocity probability distribution function (pdf) of the particle is hence a Gaussian with zero-mean and variance $T_0 = D/\gamma$. Nevertheless, for our purpose, we distinguish the thermostats and we focus on the heat flowing from one thermostat (say for example thermostat 1) to the particle over a time duration t. This quantity is exactly the total work performed by the thermostat, and it reads:

$$Q_i = \int_0^t \mathrm{d}\tau\, v(\tau)(\xi_i(\tau) - \gamma_i v(\tau)) \ , \tag{3}$$

where $i = 1, 2$. The pdf of this integrated injected power $P(Q_1, t)$ is the central object of our note. The Fluctuation Relation, applied without care, states without restriction

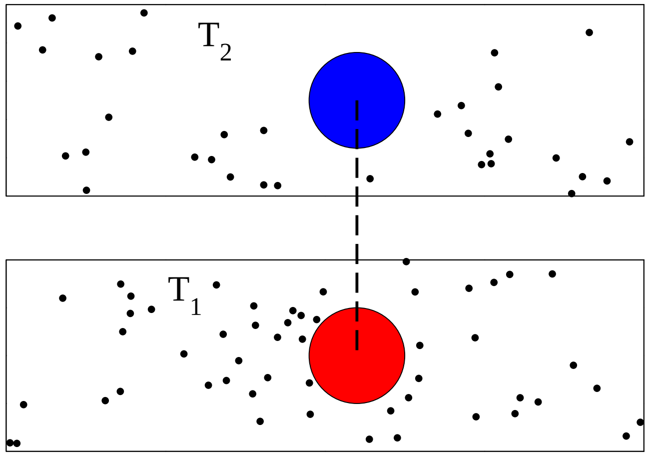

Figure 1. (color online) Sketch of a model, inspired by [9] described by the Langevin equation (1). The two particles are constrained to move together along the horizontal axis, and are in two heat baths at different temperatures.

that for the fluctuating time averaged flux $q = Q_1/t$, the large deviation function (ldf) $\pi(q)$ defined as

$$\pi(q) = \lim_{t\to\infty} \frac{1}{t} \ln P(q\,t, t) \tag{4}$$

verifies the symmetry property

$$\pi(q) - \pi(-q) = \epsilon q \ . \tag{5}$$

This is the Fluctuation Relation (FR). In Eq. (5), the constant $\epsilon = \frac{1}{T_2} - \frac{1}{T_1}$ plays the role of an external field driving the heat flux. In the following, we will also consider a restriction of the relation (5) to a finite interval (i.e. for $|q| < q^*$, where q^* is a positive constant), in analogy with deterministic systems [13, 8] and stochastic systems [7]. We will refer to this last relation as "Extended Fluctuation Relation" (EFR), from the terminology of [7]. Usually the Fluctuation Relation is supposed to be verified by the entropy flux $\mathcal{S} = Q_1/T_1 + Q_2/T_2$, which differs from $\epsilon\, Q_1$ only by a total time difference, and hence, following [8], Q_1 should, at least, verify an Extended Fluctuation Relation.

We now wish to explicitly determine $P(Q_1, t)$ at all time and investigate the properties of the large deviation function. The techniques used are similar to those employed by Farago [14]. We first introduce the joint probability $\rho(v, Q_1, t)$ that the particle has a velocity v and a given value of Q_1 at a time t. The pdf $P(Q_1, t)$ is obtained by integrating ρ over the velocity v. We also define the Laplace Transform

$$\hat{\rho}(v, \lambda, t) = \int \mathrm{d}Q_1\, \mathrm{e}^{-\lambda Q_1} \rho(v, Q_1, t) \ , \tag{6}$$

which verifies: (i) $\hat{\rho}(v, 0, t) = f(v, t)$ with $f(v, t)$ the velocity pdf of the brownian particle, and (ii) $\hat{P}(\lambda, t) = \int \mathrm{d}v \hat{\rho}(v, \lambda, t)$, with $\hat{P}(\lambda, t)$ the Laplace Transform of $P(Q_1, t)$. The pdf $\hat{\rho}(v, \lambda, t)$ verifies a Fokker-Planck Equation (FPE):

$$\frac{\partial}{\partial t} \hat{\rho}(v, \lambda, t) = L_\lambda \hat{\rho}(v, \lambda, t) \ , \tag{7}$$

where ‡

$$L_\lambda = D\frac{\partial^2}{\partial v^2} + (\gamma + 2\lambda D_1)\frac{\partial}{\partial v}v + (D_1\lambda^2 + \gamma_1\lambda)v^2 - D_1\lambda \; . \tag{8}$$

In order to get the solution of the above FPE we first note that the eigenvalue equation

$$L_\lambda f_n(v,\lambda) = \mu_n(\lambda) f_n(v,\lambda) \tag{9}$$

is solved by:

$$\mu_n(\lambda) = \frac{\gamma}{2}(1 - (1+2n)\eta) \; , \tag{10}$$

$$f_n(v,\lambda) = \frac{\mathrm{e}^{-\frac{v^2}{2T(\lambda)}}}{\sqrt{2\pi T(\lambda)}} H_n\left(\frac{v}{\sqrt{2T^*(\lambda)}}\right) / \sqrt{2^n n!} \; , \tag{11}$$

where:

$$\eta = \sqrt{1 + \frac{4\lambda}{\gamma^2}(\gamma_2 D_1 - \gamma_1 D_2 - \lambda D_1 D_2)} \; , \tag{12}$$

$$T(\lambda) = \frac{2D}{\gamma(1+\eta) + 2\lambda D_1} \; , \quad T^*(\lambda) = T_0/\eta \; , \tag{13}$$

and where $H_n(x)$ denotes the Hermite polynomial of order n. We remark that the largest eigenvalue $\mu_0(\lambda)$ presents the symmetry

$$\mu_0(\lambda) = \mu_0(\epsilon - \lambda) \; , \tag{14}$$

with $\epsilon = 1/T_2 - 1/T_1$. Should $\pi(q)$ be the Legendre Transform of $\mu_0(\lambda)$, this last relation would exactly yield (5) [6]. The solution of (7) for a given initial condition is hence easily obtained as:

$$\hat{\rho}(v,\lambda,t|v_0) = \sum_{n=0}^{\infty} \mathrm{e}^{\mu_n(\lambda)t} C_n(v,\lambda|v_0) f_n(v,\lambda) \; , \tag{15}$$

where $C_n(v,\lambda|v_0)$ is the projection of the n-th eigenfunction onto the initial state, which has been chosen to be a Dirac function centered in $v = v_0$. In order to simplify the notations we will set all the scales to unity (i.e. $\gamma = D = T_0 = 1$), and introduce

$$\tilde{\gamma}_1 = \frac{\gamma_1}{\gamma} = \frac{1+\Delta\gamma}{2} \; , \quad \tilde{\gamma}_2 = \frac{\gamma_2}{\gamma} = \frac{1-\Delta\gamma}{2} \; , \tag{16}$$

$$\tilde{D}_1 = \frac{D_1}{D} = \frac{1+\Delta D}{2} \; , \quad \tilde{D}_2 = \frac{D_2}{D} = \frac{1-\Delta D}{2} \; , \tag{17}$$

where both $\Delta\gamma$ and ΔD take values between -1 and 1. Thus, when $T_1 = T_2$ one has that $\Delta\gamma = \Delta D$. Finally, integrating $\hat{\rho}$ over the velocity, one obtains the expression of $\hat{P}(\lambda,t)$ for a given initial velocity v_0:

$$\hat{P}(\lambda,t|v_0) = \mathrm{e}^{\frac{t}{2}}\left(\cosh(\eta t) + (\lambda(1+\Delta D)+1)\frac{\sinh(\eta t)}{\eta}\right)^{-\frac{1}{2}} \exp\left(\frac{v_0^2}{2}\left(\frac{\lambda(1+\Delta\gamma+(1+\Delta D)\lambda)}{1+\lambda(1+\Delta D)+\eta\coth(\eta t)}\right)\right) . \tag{18}$$

‡ A detailed derivation of this operator for a slightly different system is given in: P. Visco, A. Puglisi, A. Barrat, E. Trizac and F. van Wijland, submitted to J. Stat. Phys, `cond-mat/0509487`.

The long time behavior of $\hat{P}(\lambda, t)$ is clearly dominated by $\hat{P}(\lambda, t) \sim \mathrm{e}^{\mu_0(\lambda)t}$, with $\mu_0(\lambda)$ the largest eigenvalue of L_λ. This result was already found in [1]. The expression of μ_0 presents two cuts in the real axis for $\lambda > \lambda_+$ and $\lambda < \lambda_-$, with:

$$\lambda_\pm = \frac{\Delta D - \Delta\gamma}{1 - \Delta D^2} \pm \sqrt{\frac{1 - 2\Delta D \Delta\gamma + \Delta\gamma^2}{(1 - \Delta D^2)^2}} \ . \tag{19}$$

Nonetheless, it is possible to see that the subleading prefactor entering in expression (18) presents an extra cut for $\lambda < \lambda_-^*$, where, in the infinite time limit,

$$\lambda_-^* = -\frac{1 + \Delta\gamma}{1 + \Delta D} \ . \tag{20}$$

Note that this cut exists only for $\Delta\gamma > 0$, and implies that the right tail of the large deviation function of Q_1 will present an exponential decay, with a slope different than the one predicted by the Legendre Transform of μ_0. The quantitative details on how this extra cut will affect $\pi(q)$ will be given later. Let us now give some comments on this issue. The energy balance equation for this particular system can be written as:

$$\Delta E(t) = E(t) - E(0) = Q_1 + Q_2 \ , \tag{21}$$

where Q_2 denotes the work performed by the thermostat at temperature T_2 on the particle, and is defined by Eq (3). Physical intuition would suggest that for very long times, since the Q_i's are extensive in time while the "boundary term" ΔE is not, the latter does not come into play when determining the large deviation of, say, Q_1, and in particular that Q_1 and $-Q_2$ have the same large deviation functions. However, in several examples [14, 15, 7, 16, 8] it has been noted that, if the boundary term distribution has exponentially (or slower) decreasing tails then, even in the infinite time limit, it can have a fluctuation of order t, and hence is no more negligible. Clearly in our case, since the velocity pdf is Gaussian, the energy has exponential tails. If the initial condition v_0 is fixed, then ΔE has only a right exponential tail, which may affect the right tail of the large deviation function of Q_1. This is precisely the reason for the presence of our extra cut. Besides, if the initial condition is sampled on the stationary velocity pdf, the boundary term ΔE will have two exponential tails, and therefore two extra cuts may appear in the λ complex plane. When the initial condition is sampled in the stationary state, one finds:

$$\hat{P}(\lambda) = \int \mathrm{d}v_0 \, \mathrm{e}^{-\frac{v_0^2}{2}} \hat{P}(\lambda|v_0) = \mathrm{e}^{\frac{t}{2}} \times \left(\cosh(\eta t) + \frac{\sinh(\eta t)}{\eta} (1 - \lambda(\Delta\gamma + \Delta D(\lambda - 1) + \lambda)) \right)^{\frac{1}{2}} . \tag{22}$$

In the infinite time limit this last expression still presents the λ_-^* extra cut for $\Delta\gamma > 0$. Moreover, a new cut appears for $\Delta D > \Delta\gamma/2$ and for $\lambda > \lambda_+^*$ with

$$\lambda_+^* = \frac{1 + 2\Delta D - \Delta\gamma}{1 + \Delta D} \ . \tag{23}$$

These cuts are schematized in a diagram in figure 2.

The Laplace Transform can be safely inverted using the Legendre Transform only in the region in which:

$$\max(\lambda_-, \lambda_-^*) < \lambda < \min(\lambda_+, \lambda_+^*) \ . \tag{24}$$

The Legendre Transform gives hence in this region:

$$\pi_c(q) = -\frac{1 - \Delta D^2 + 2q(\Delta\gamma - \Delta D) + \sqrt{(1 + \Delta\gamma^2 - 2\Delta\gamma\Delta D)(1 + 4q^2 - \Delta D^2)}}{2(1 - \Delta D^2)} \ . \tag{25}$$

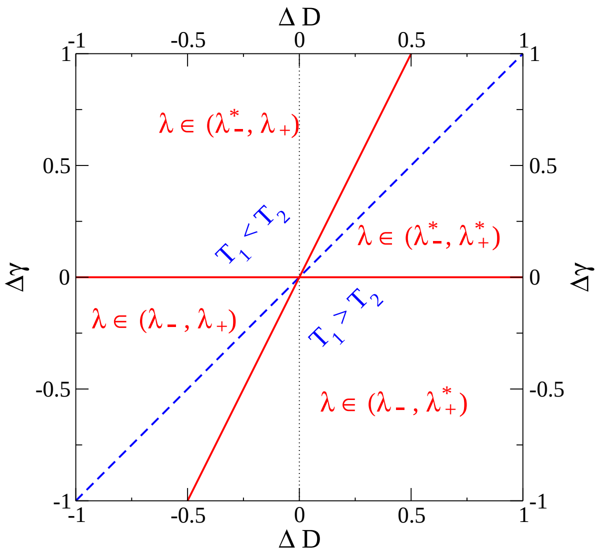

Figure 2. (color online) Diagram for the extra cuts in the real λ axis. The solid lines separate the regions of the parameter space $(\Delta\gamma, \Delta D)$ for which $\hat{P}(\lambda)$ has different domains of definition in the λ-real axis. The dashed line is the line where $T_1 = T_2$.

If the bounds of $\hat{P}(\lambda)$ are (on the real axis) λ_+ and λ_- the above expression is valid for any q, and the Fluctuation Relation holds. Besides, if the left (right) cut begins at λ_-^* (λ_+^*), the Legendre Transform of $\mu_0(\lambda)$ is valid only for $q < q_+ = \mu_0'(\lambda_-^*)$ ($q > q_- = \mu_0'(\lambda_+^*)$). In this case the expression of $\pi(q)$ outside the interval (q_-, q_+) is a straight line $\pi(q) = \alpha + \beta q$, and the coefficients α and β can be obtained using that both $\pi(q)$ and $\pi'(q)$ must be continuous functions of q (this is not evident for the derivative $\pi'(q)$, but it is effectively the case in [14], where essentially the same model has been worked out). For example in the region $\Delta\gamma > 0$ and $\Delta D > \Delta\gamma/2$ one has:

$$\pi(q) = \begin{cases} \pi_l(q) & q < q_- \\ \pi_c(q) & q_- < q < q_+ \\ \pi_r(q) & q > q_+ \ , \end{cases} \tag{26}$$

with

$$q_- = \frac{\Delta D}{2} - \frac{1}{2(2\Delta D - \Delta\gamma)} \ , \quad q_+ = \frac{1}{2\Delta\gamma} - \frac{\Delta D}{2} \ , \tag{27}$$

$$\pi_l(q) = -\frac{(1 + 2\Delta D - \Delta\gamma)(1 + \Delta D - 2q)}{2(1 + \Delta D)} \ , \tag{28}$$

$$\pi_r(q) = -\frac{(1 + \Delta\gamma)(1 + \Delta D + 2q)}{2(1 + \Delta D)} \ . \tag{29}$$

The behavior of $\pi(q)$ in the others regions can be obtained in a similar fashion. If an extra cut starts at λ_-^*, then for $q > q_+$ the ldf $\pi(q)$ is equal to $\pi_r(q)$. Analogously, if an extra cut begins at λ_+^*, then for $q < q_-$ one has $\pi(q) = \pi_l(q)$. In all the other cases $\pi(q) = \pi_c(q)$. The Fluctuation Relation (5) is only satisfied in the case for which $\pi(q) = \pi_c(q)$. The Extended Fluctuation Relation is satisfied in the cases where

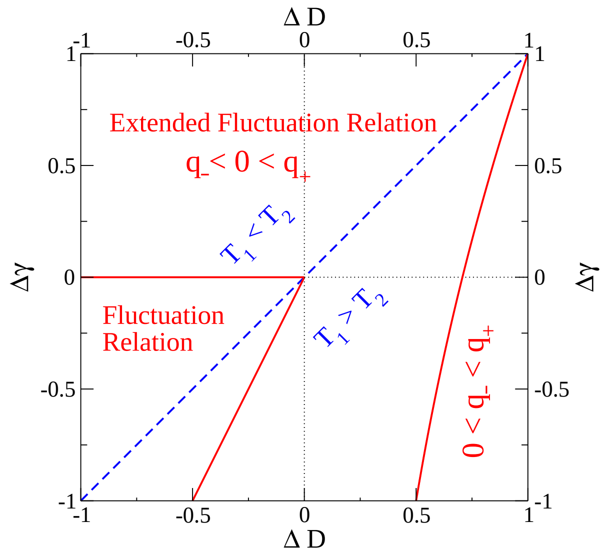

Figure 3. (color online) Diagram schematizing the domain of validity of the Fluctuation Relation and of the Extended Fluctuation Relation (see text for details).

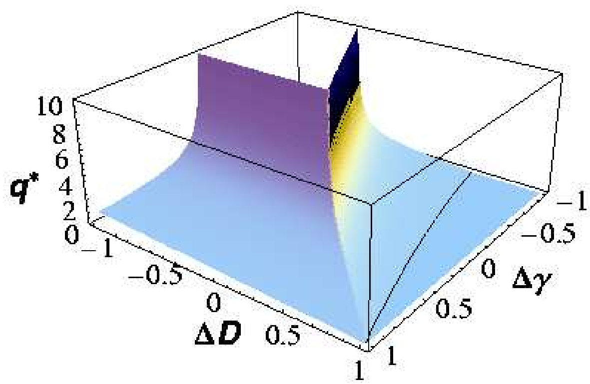

Figure 4. (color online) Three dimensional plot of q^*, as a function of the system's parameters. In the region in which $q^* = \infty$ the FR is verified. The solid line delimitates the region in which $q^* = 0$, where the EFR fails.

$q_- < 0 < q_+$ (see the diagram in Fig 3). In this case q^* is the minimum between $|q_-|$ and $|q_+|$, and is plotted in Fig 4. Surprisingly it also happens that, in a in a given region of the parameters' space (i.e. when $\Delta\gamma < 2\Delta D - 1/\Delta D$) one has that $0 < q_- < q_+$. In this case $q^* = 0$ and both the FR and the EFR break down. In particular it is found, for small values of q, that:

$$\pi(q) - \pi(-q) = \pi_l(q) - \pi_l(-q) = \zeta q\,, \qquad |q| < q_- \tag{30}$$

with $\zeta = 4/T_0 - 2/T_1$ (an illustration is given in Fig 5).

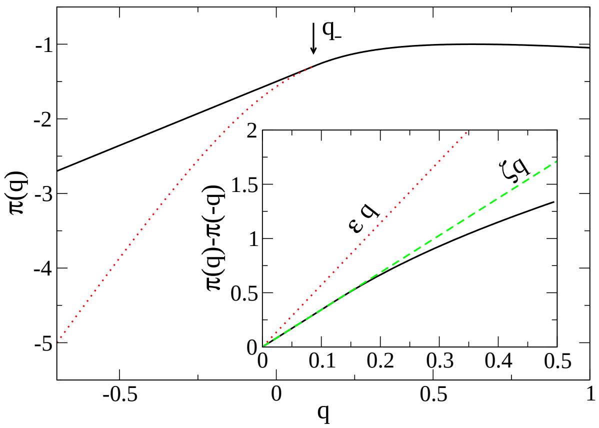

Figure 5. Plot of the large deviation function $\pi(q)$ for $\Delta D = 0.75$ and $\Delta\gamma = -0.5$. The (red) dotted line shows $\pi_c(q)$, for which the Fluctuation Relation holds. The inset shows the plot of $\pi(q) - \pi(-q)$. The (red) dotted line is a straight line of slope ϵ, while the (green) dashed line has a slope ζ (see text for details).

We now turn on some remarks concerning the importance of initial conditions. If the two temperatures T_1 and T_2 are equal, it is clear that the average flux $\langle Q_1 \rangle = 0$, with $\pi(q) = \pi(-q)$. Surprisingly, if the ldf $\pi(q|v_0)$ is measured for $\Delta\gamma > 0$ (and $T_1 = T_2$), with a fixed initial condition v_0, one would see that $\pi(q|v_0) \neq \pi(-q|v_0)$ (because of the right extra cut), which would lead to the wrong impression that there is a nonzero flux from one thermostat to the other, even if they are at the same temperature. Of course, if $\pi(q)$ is measured sampling the initial conditions in the stationary state, a new extra cut appears, restoring the symmetry $\pi(q) = \pi(-q)$. This can be understood with the following remark. The right tail of $\pi(q|v_0)$ is somehow dominated by the events with an "energetic final condition" (cf. also [14]). The bias enforced by the fixed initial condition (even in the case where $v_0 = \langle v \rangle = 0$), forbids the occurrence of "energetic initial conditions", which would balance (on average) the energetic final conditions, and leads then to the appearance of an unphysical flux.

Our results answer some issues raised in the recent developments of the theory of nonequilibrium fluctuations. In particular, we have provided the confirmation that if two quantities, both extensive in time (as e.g. $Q_1(t)$ and $Q_2(t)$), differ one from the other by a "boundary term" (as $\Delta E(t)$), whose pdf has tails with exponential decay, they do not have the same large deviation function. This also leads to a small restriction to the validity of the very general result obtained in [5, 6]. Furthermore, our results clearly show that, even if the Fluctuation Relation (5) is broken, the largest eigenvalue $\mu_0(\lambda)$ always displays the symmetry property analogous to (14). While the latter result is obviously mathematically robust, this is also the most relevant physics-wise, since for small fluctuations around the average and for small nonequilibrium drive, it leads to the well-known fluctuation-dissipation theorem.

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